```
     (FILE 'HOME' ENTERED AT 10:55:29 ON 17 DEC 2003)

     FILE 'USPATFULL, CAPLUS' ENTERED AT 10:55:48 ON 17 DEC 2003
               ACTIVATE L09980406/L
              ---------
L1              STR
L2   (         11)SEA FILE=REGISTRY SSS FUL L1
L3   (         30)SEA FILE=CAPLUS ABB=ON  PLU=ON  L2
L4   (         14)SEA FILE=CAPLUS ABB=ON  PLU=ON  L2/USES OR L2/BIOL
L5   (          0)SEA FILE=CAPLUS ABB=ON  PLU=ON  L4 AND HAIR
L6   (          0)SEA FILE=CAPLUS ABB=ON  PLU=ON  L4 AND THYROIDR
L7   (         13)SEA FILE=CAPLUS ABB=ON  PLU=ON  L4 AND THYROID
L8   (          0)SEA FILE=CAPLUS ABB=ON  PLU=ON  L4 AND ALOPECIA
L9   (          0)SEA FILE=CAPLUS ABB=ON  PLU=ON  L4 AND BALD?
L10  (          3)SEA FILE=USPATFULL ABB=ON  PLU=ON  L2
L11  (          2)SEA FILE=CAPLUS ABB=ON  PLU=ON  40487-99-8/BIOL
L12  (          0)SEA FILE=TOXCENTER ABB=ON  PLU=ON  40487-99-8/BIOL
L13  (          2)SEA 40487-99-8/BIOL
L14  (          2)SEA FILE=CAPLUS ABB=ON  PLU=ON  40487-99-8
L15  (          0)SEA FILE=TOXCENTER ABB=ON  PLU=ON  40487-99-8
L16  (          2)SEA 40487-99-8
L17  (          1)SEA FILE=CAPLUS ABB=ON  PLU=ON  27486-96-0
L18  (          0)SEA FILE=TOXCENTER ABB=ON  PLU=ON  27486-96-0
L19  (          1)SEA 27486-96-0
L20  (         12)SEA FILE=CAPLUS ABB=ON  PLU=ON  52050-08-5 OR 40487-99-8 OR L17
L21  (          1)SEA FILE=TOXCENTER ABB=ON  PLU=ON  52050-08-5 OR 40487-99-8 OR
L22  (         13)SEA 52050-08-5 OR 40487-99-8 OR L19
L23  (         10)SEA FILE=CAPLUS ABB=ON  PLU=ON  CARDIAC SPARING
L24  (          8)SEA FILE=USPATFULL ABB=ON  PLU=ON  CARDIAC SPARING
L25  (         18)SEA CARDIAC SPARING
L26  (         19)SEA FILE=CAPLUS ABB=ON  PLU=ON  CARDIAC (5A) SPARING
L27  (         35)SEA FILE=USPATFULL ABB=ON  PLU=ON  CARDIAC (5A) SPARING
L28  (         54)SEA CARDIAC (5A) SPARING
L29  (          4)SEA FILE=CAPLUS ABB=ON  PLU=ON  THYROID AND L26
L30  (          5)SEA FILE=USPATFULL ABB=ON  PLU=ON  THYROID AND L27
L31  (          9)SEA THYROID AND L28
L32  (          0)SEA FILE=CAPLUS ABB=ON  PLU=ON  L20 AND L26
L33  (          0)SEA FILE=USPATFULL ABB=ON  PLU=ON  L22 AND L27
L34  (          0)SEA L22 AND L28
L35  (          0)SEA FILE=CAPLUS ABB=ON  PLU=ON  L20 AND (CARDIAC)
L36  (          0)SEA FILE=USPATFULL ABB=ON  PLU=ON  L22 AND (CARDIAC)
L37  (          0)SEA L22 AND (CARDIAC)
L38  (          1)SEA FILE=CAPLUS ABB=ON  PLU=ON  L20 AND (HEART OR PRESSURE)
L39  (          0)SEA FILE=USPATFULL ABB=ON  PLU=ON  L22 AND (HEART OR PRESSURE)
L40  (          1)SEA L22 AND (HEART OR PRESSURE)
L41  (          1)SEA FILE=CAPLUS ABB=ON  PLU=ON  L20 AND (HEART OR PRESSURE)
L42  (          0)SEA FILE=TOXCENTER ABB=ON  PLU=ON  L21 AND (HEART OR PRESSURE)
L43  (          1)SEA L40
              ---------

     FILE 'REGISTRY, USPATFULL, CAPLUS' ENTERED AT 10:56:17 ON 17 DEC 2003
L44             1 FILE REGISTRY
L45            11 FILE REGISTRY

     FILE 'CAPLUS, USPATFULL, TOXCENTER' ENTERED AT 11:02:03 ON 17 DEC 2003
L46            30 FILE CAPLUS
L47             3 FILE USPATFULL
L48             5 FILE TOXCENTER
     TOTAL FOR ALL FILES
L49            38 S L45
L50             2 FILE CAPLUS
L51             0 FILE USPATFULL
L52             0 FILE TOXCENTER
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     TOTAL FOR ALL FILES
L53            2 S TRIMETHYLTHYRONINE
L54            4 FILE CAPLUS
L55            0 FILE USPATFULL
L56            1 FILE TOXCENTER
     TOTAL FOR ALL FILES
L57            5 S TRIMETHYL(3A)THYRONINE
L58        18002 FILE CAPLUS
L59         3924 FILE USPATFULL
L60         3208 FILE TOXCENTER
     TOTAL FOR ALL FILES
L61        25134 S (L-TYROSINE) OR (L(1W) TYROSINE)
L62           47 FILE CAPLUS
L63           33 FILE USPATFULL
L64            6 FILE TOXCENTER
     TOTAL FOR ALL FILES
L65           86 S L61 (5A) (DIMETHYL)
L66          100 FILE CAPLUS
L67          104 FILE USPATFULL
L68            9 FILE TOXCENTER
     TOTAL FOR ALL FILES
L69          213 S L61 (5A) (DIMETHYL?)
L70            5 FILE CAPLUS
L71            8 FILE USPATFULL
L72            1 FILE TOXCENTER
     TOTAL FOR ALL FILES
L73           14 S L69 (5A) (HYDROXY?)
L74        19717 FILE CAPLUS
L75         2175 FILE USPATFULL
L76         8512 FILE TOXCENTER
     TOTAL FOR ALL FILES
L77        30404 S 52050-08-5/RN OR ?THYRONINE? OR 52050-08-5
L78           61 FILE CAPLUS
L79          495 FILE USPATFULL
L80           38 FILE TOXCENTER
     TOTAL FOR ALL FILES
L81          594 S L77 AND (HAIR? OR ALOPECIA OR BALD?)

     FILE 'REGISTRY' ENTERED AT 11:09:46 ON 17 DEC 2003
L82            1 S THYRONINE/CN

     FILE 'CAPLUS, USPATFULL, TOXCENTER' ENTERED AT 11:10:13 ON 17 DEC 2003
L83            8 FILE CAPLUS
L84          436 FILE USPATFULL
L85            3 FILE TOXCENTER
     TOTAL FOR ALL FILES
L86          447 S L81 AND (METHYL?)
L87            9 FILE CAPLUS
L88          428 FILE USPATFULL
L89            5 FILE TOXCENTER
     TOTAL FOR ALL FILES
L90          442 S L81 AND (?METHYL)
L91           10 FILE CAPLUS
L92          445 FILE USPATFULL
L93            7 FILE TOXCENTER
     TOTAL FOR ALL FILES
L94          462 S L86 OR L90

     FILE 'REGISTRY' ENTERED AT 11:17:55 ON 17 DEC 2003
L95            1 S 6893-02-3/RN
                 SET NOTICE 1 DISPLAY
                 SET NOTICE LOGIN DISPLAY

     FILE 'CAPLUS, USPATFULL, TOXCENTER' ENTERED AT 11:19:00 ON 17 DEC 2003
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L96        31768 FILE CAPLUS
L97        58023 FILE USPATFULL
L98        11948 FILE TOXCENTER
     TOTAL FOR ALL FILES
L99       101739 S TRIIODOTHYRONINE OR (L-T3) OR (L(1W) T3) OR T3 OR (TRIIODO (5
L100     2550638 FILE CAPLUS
L101      873754 FILE USPATFULL
L102      497113 FILE TOXCENTER
     TOTAL FOR ALL FILES
L103     3921505 S SUBSTITUT? OR ALKYLAT? OR METHYL?
L104        1344 FILE CAPLUS
L105        1011 FILE USPATFULL
L106         437 FILE TOXCENTER
     TOTAL FOR ALL FILES
L107        2792 S L99 (2S) (L103 OR (FREE (3A) IODINE))
L108        1156 FILE CAPLUS
L109        1010 FILE USPATFULL
L110         348 FILE TOXCENTER
     TOTAL FOR ALL FILES
L111        2514 S L99 (1S) (L103 OR (FREE (3A) IODINE))
L112          14 FILE CAPLUS
L113           2 FILE USPATFULL
L114           9 FILE TOXCENTER
     TOTAL FOR ALL FILES
L115          25 S L99 (1S) ((FREE (3A) IODINE))

     FILE 'REGISTRY' ENTERED AT 11:28:03 ON 17 DEC 2003

     FILE 'CAPLUS, USPATFULL, TOXCENTER' ENTERED AT 11:28:06 ON 17 DEC 2003

     FILE 'REGISTRY' ENTERED AT 11:28:19 ON 17 DEC 2003

     FILE 'CAPLUS, USPATFULL, TOXCENTER' ENTERED AT 11:28:20 ON 17 DEC 2003

     FILE 'REGISTRY' ENTERED AT 11:28:26 ON 17 DEC 2003

     FILE 'CAPLUS, USPATFULL, TOXCENTER' ENTERED AT 11:28:28 ON 17 DEC 2003

     FILE 'REGISTRY' ENTERED AT 11:28:33 ON 17 DEC 2003

     FILE 'CAPLUS, USPATFULL, TOXCENTER' ENTERED AT 11:28:35 ON 17 DEC 2003

     FILE 'REGISTRY' ENTERED AT 11:28:41 ON 17 DEC 2003

     FILE 'CAPLUS, USPATFULL, TOXCENTER' ENTERED AT 11:28:42 ON 17 DEC 2003
L116           2 FILE CAPLUS
L117           1 FILE USPATFULL
L118           0 FILE TOXCENTER
     TOTAL FOR ALL FILES
L119           3 S L99 (1S) ((FREE (3A) HALOGEN?))
L120           2 FILE CAPLUS
L121           1 FILE USPATFULL
L122           0 FILE TOXCENTER
     TOTAL FOR ALL FILES
L123           3 S L119 NOT L115

     FILE 'USPATFULL, CAPLUS' ENTERED AT 11:40:44 ON 17 DEC 2003
L124         343 FILE USPATFULL
L125       17177 FILE CAPLUS
     TOTAL FOR ALL FILES
L126       17520 S 6893-02-3/RN OR 6893-02-3
L127       58067 FILE USPATFULL
L128       32491 FILE CAPLUS
     TOTAL FOR ALL FILES
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L129      90558 S L99 OR L126
L130          3 FILE USPATFULL
L131         99 FILE CAPLUS
     TOTAL FOR ALL FILES
L132        102 S L129 (2S) (FREE (5A) (HALOGEN OR IODO?))
L133          2 FILE USPATFULL
L134         99 FILE CAPLUS
     TOTAL FOR ALL FILES
L135        101 S L132 NOT 119
L136          2 FILE USPATFULL
L137         98 FILE CAPLUS
     TOTAL FOR ALL FILES
L138        100 S L135 NOT L115
                SAVE ALL L09980406/L

     FILE 'EMBASE, MEDLINE, BIOSIS, SCISEARCH' ENTERED AT 11:54:24 ON 17 DEC
     2003
L139      30070 FILE EMBASE
L140      33763 FILE MEDLINE
L141      32585 FILE BIOSIS
L142      18104 FILE SCISEARCH
     TOTAL FOR ALL FILES
L143     114522 S L129
L144          7 FILE EMBASE
L145          4 FILE MEDLINE
L146          4 FILE BIOSIS
L147          4 FILE SCISEARCH
     TOTAL FOR ALL FILES
L148         19 S L143 (1S) ((ME OR METHYL OR ALKYL) (2W) SUBSTITUT?)
L149         11 DUP REM L148 (8 DUPLICATES REMOVED)

     FILE 'STNGUIDE' ENTERED AT 12:02:03 ON 17 DEC 2003
                SAVE ALL L099804
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L115 ANSWER 14 OF 25 CAPLUS COPYRIGHT 2003 ACS ón STN

AB Iodide does not exchange with iodinated thyronines under conditions which assure the absence of **free iodine**. Iodine exchanges readily with both thyroxine and **triiodothyronine** in synthetic soln. at physiol. pH. The rate of exchange at 10-4M far exceeds that of substitution under the same conditions. The distribution of radioactivity is proportional to the molar ratios of the products, i.e., quant. Labeling by exchange involves only the "prime" positions. A new solvent is described which provides excellent resolution of the compds. encountered; it is tert-AmOH satd. with 2N NH4OH.

ACCESSION NUMBER:	1955:46576 CAPLUS
DOCUMENT NUMBER:	49:46576
ORIGINAL REFERENCE NO.:	49:9070a-c
TITLE:	The exchange of iodine with thyroxine homologs
AUTHOR(S):	Gleason, Geoffrey I.
CORPORATE SOURCE:	Abbott Labs., Oak Ridge, TN
SOURCE:	Journal of Biological Chemistry (1955), 213, 837-41 CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE:	Journal
LANGUAGE:	Unavailable

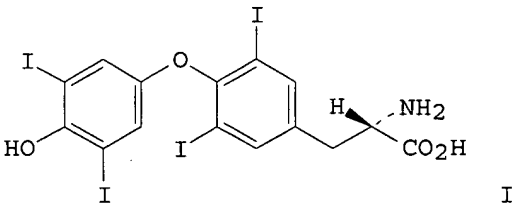
AN 72:133162 CA
TI Thyroxine analogs. XVIII. 3,5-Dialkyl-3'-halo-DL-thyronines and their 3'-methyl and 4'-amino analogs
AU Jorgensen, Eugene C.; Wright, Jeremy
CS Sch. of Pharm., Univ. of California, San Francisco, CA, USA
SO Journal of Medicinal Chemistry (1970), 13(3), 367-70
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
CC 34 (Synthesis of Amino Acids, Peptides, and Proteins)
AB The synthesis of 3,5-diisopropyl- and 3,5-di-secbutyl-DL-thyronines and their 4'-amino, 3'-bromo, and 3'-iodo analogs is reported. 3,5-Diisopropyl-3'-methyl-DL-thyronine was also prepd. All 3,5-diisopropyl-and 3,5-di-sec-butyl-DL-thyronines and their derivs. and analogs were inactive as thyromimetics in the rat antigoiter test. The 3,5-dialkyl-3'-iodo-DL-thyronines of this series were also inactive as thyroxine-like agents by the heart-rate and tadpole metamorphosis methods. All analogs tested as thyroxine antagonists by the antigoiter assay were inactive.
ST thyroxine analogs thyronines; thyronines thyroxine analogs
IT Molecular structure-biological activity relationships
(thyroxic, of thyronine alkyl derivs.)
IT Thyronine, 3,5-dialkyl-3'-halo derivs., DL-
Thyroxine, ar-alkyl analogs, DL-
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 17944-26-2P 19288-25-6P 25806-78-4P 25849-86-9P 27144-21-4P
27144-22-5P 27144-23-6P 27144-24-7P 27144-25-8P 27144-26-9P
27144-27-0P 27144-28-1P 27144-29-2P 27192-12-7P 27192-13-8P
27486-96-0P 27486-97-1P 27486-98-2P 27487-00-9P 27487-02-1P
27487-03-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

AN 72:133162 CA
TI Thyroxine analogs. XVIII. 3,5-Dialkyl-3'-halo-DL-thyronines and their 3'-methyl and 4'-amino analogs
AU Jorgensen, Eugene C.; Wright, Jeremy
CS Sch. of Pharm., Univ. of California, San Francisco, CA, USA
SO Journal of Medicinal Chemistry (1970), 13(3), 367-70
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
CC 34 (Synthesis of Amino Acids, Peptides, and Proteins)
AB The synthesis of 3,5-diisopropyl- and 3,5-di-secbutyl-DL-thyronines and their 4'-amino, 3'-bromo, and 3'-iodo analogs is reported. 3,5-Diisopropyl-3'-methyl-DL-thyronine was also prepd. All 3,5-diisopropyl-and 3,5-di-sec-butyl-DL-thyronines and their derivs. and analogs were inactive as thyromimetics in the rat antigoiter test. The 3,5-dialkyl-3'-iodo-DL-thyronines of this series were also inactive as thyroxine-like agents by the heart-rate and tadpole metamorphosis methods. All analogs tested as thyroxine antagonists by the antigoiter assay were inactive.
ST thyroxine analogs thyronines; thyronines thyroxine analogs
IT Molecular structure-biological activity relationships
(thyroxic, of thyronine alkyl derivs.)
IT Thyronine, 3,5-dialkyl-3'-halo derivs., DL-
Thyroxine, ar-alkyl analogs, DL-
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 17944-26-2P 19288-25-6P 25806-78-4P 25849-86-9P 27144-21-4P
27144-22-5P 27144-23-6P 27144-24-7P 27144-25-8P 27144-26-9P
27144-27-0P 27144-28-1P 27144-29-2P 27192-12-7P 27192-13-8P
27486-96-0P 27486-97-1P 27486-98-2P 27487-00-9P 27487-02-1P
27487-03-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

AN 72:133162 CA
TI Thyroxine analogs. XVIII. 3,5-Dialkyl-3'-halo-DL-thyronines and their 3'-methyl and 4'-amino analogs
AU Jorgensen, Eugene C.; Wright, Jeremy
CS Sch. of Pharm., Univ. of California, San Francisco, CA, USA
SO Journal of Medicinal Chemistry (1970), 13(3), 367-70
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
CC 34 (Synthesis of Amino Acids, Peptides, and Proteins)
AB The synthesis of 3,5-diisopropyl- and 3,5-di-secbutyl-DL-thyronines and their 4'-amino, 3'-bromo, and 3'-iodo analogs is reported. 3,5-Diisopropyl-3'-methyl-DL-thyronine was also prepd. All 3,5-diisopropyl-and 3,5-di-sec-butyl-DL-thyronines and their derivs. and analogs were inactive as thyromimetics in the rat antigoiter test. The 3,5-dialkyl-3'-iodo-DL-thyronines of this series were also inactive as thyroxine-like agents by the heart-rate and tadpole metamorphosis methods. All analogs tested as thyroxine antagonists by the antigoiter assay were inactive.
ST thyroxine analogs thyronines; thyronines thyroxine analogs
IT Molecular structure-biological activity relationships
(thyroxic, of thyronine alkyl derivs.)

AN 78:154689 CA
TI Thyromimetic activity of 3,5,3'-trimethyl-L-thyronine
AU Jorgensen, Eugene C.; Block, Paul, Jr.
CS Sch. Ppharm., Univ. California, San Francisco, CA, USA
SO Journal of Medicinal Chemistry (1973), 16(3), 306-7
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
CC 1-3 (Pharmacodynamics)
Section cross-reference(s): 2
AB 3,5,3'-Trimethyl-L-thyronine (I) [40487-99-8] showed about 2% of the activity of L-thyroxine in reversing thiouracil-induced goiter in rats. I was thus the 1st reported nonhalogenated compd. having thyroid hormone activity. I was prepd. by the general method of P. Block Jr. and D. H. Coy (1972).
ST methylthyronine thyroid hormone activity; thyroxine analog synthesis
IT Thyroid hormones
RL: BIOL (Biological study)
(trimethylthyronine)
IT Goiter
(trimethylthyronine reversal of)
IT 40487-99-8
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(thyromimetic activity of)

AN 87:16156 CA
TI Thyroxine analogs. 23. Quantitative structure-activity correlation studies of in vivo and in vitro thyromimetic activities
AU Dietrich, Stephen W.; Bolger, Michael B.; Kollman, Peter A.; Jorgensen, Eugene C.
CS Sch. Pharm., Univ. California, San Francisco, CA, USA
SO Journal of Medicinal Chemistry (1977), 20(7), 863-80
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
CC 2-3 (Hormone Pharmacology)
Section cross-reference(s): 22, 34
GI



I

AB Quant. structure-activity correlation studies of thyroxine (I) [51-48-9] and 78 analogs included studies of in vivo rat antigoiter activities, and in vitro binding affinities to intact rat hepatic nuclei, solubilized rat hepatic nuclear protein receptors, and plasma protein thyroxine-binding globulin, as well as correlation between in vivo and in vitro activities. Structure-activity relations including substituent effects such as steric effects, electron donation, H bonding, ionization, and lipophilicity, as well as free energy of binding are discussed.
ST thyroxine analog structure activity; thyroid hormone analog antigoiter; thyromimetic thyroxine analog; free energy binding thyroxine analog
IT Free energy
(of binding, of thyroxine analogs to nuclear receptors, structure in relation to)
IT Substituent effect
(on thyromimetic activity of thyroid hormone analogs)
IT Molecular structure-biological activity relationship
(thyromimetic, of thyroid hormone analogs, calcn. of)
IT Thyroid hormones
(thyroxine, quant. structure-activity relations of)
IT 4299-83-6 62901-40-0 62901-41-1 62901-42-2 62901-43-3 62901-44-4 62901-45-5 62901-46-6 62901-47-7 62901-48-8 62901-51-3 62960-49-0 67737-63-7
RL: PROC (Process)
(binding of, to hepatic nuclear protein receptors, free energy of)
IT 70-39-3 4080-15-3 4299-87-0 4564-77-6 5383-39-1 39693-06-6 51725-31-6 58297-21-5 58297-22-6 62901-39-7
RL: PROC (Process)
(binding of, to hepatic nuclei, free energy of)
IT 51-48-9, biological studies 51-48-9D, analogs 534-51-0 3130-96-9 3458-13-7 4080-14-2 10439-94-8
RL: BIOL (Biological study)
(thyromimetic activity of, calcn. of)
IT 4289-12-7 4299-83-6 4299-88-1 6893-08-9 6994-12-3 7582-57-2 10468-95-8 17944-26-2 22153-98-6 25119-48-6 26384-19-0 26384-20-3 26384-21-4 35152-70-6 35152-73-9 35152-79-5 35152-81-9 37642-60-7 38896-90-1 40487-99-8 56807-75-1

60363-26-0 60497-68-9 61476-49-1 62901-23-9 62901-24-0
62901-25-1 62901-27-3 62901-28-4 62901-29-5 62901-30-8
62901-31-9 62901-32-0 62901-33-1 62901-34-2 62901-35-3
62901-36-4 62901-37-5 62901-38-6 62901-49-9 62901-50-2
62901-51-3 62901-52-4 62960-46-7 62960-48-9 62961-71-1
67737-63-7 91840-96-9
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(thyromimetic activity of, calcn. of)

AN 80:142047 CA
TI Molecular orbital studies of thyroid hormone analogs
AU Kollman, Peter A.; Murray, Wallace J.; Nuss, Merrill E.; Jorgensen, Eugene C.; Rothenberg, Steve
CS Dep. Pharm. Chem., Univ. California, San Francisco, CA, USA
SO Journal of the American Chemical Society (1973), 95(26), 8518
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
CC 6-3 (General Biochemistry)
Section cross-reference(s): 2
AB Mol. orbital calcns. on thyroxine analogs indicate that the min. energy conformation for 3,5-disubstituted compds. is an important structural feature detg. biol. activity. The proximal conformation of 3,5,3'-triiodothyronine is predicted to be very slightly (0.2 kcal/mole) more stable than the distal. The representation of the valence electrons of Cl, Br, and I with 2s- and 2p-like at. orbitals appears to give a reasonably satisfactory representation of the electronic structure of these halogen compds.
ST thyroid hormone analog conformation; thyroxine conformation; iodothyronine conformation
IT Molecular structure-biological activity relationship
(of thyroxine and triiodothyronine)
IT Conformation and Conformers
(of thyroxine and triiodothyronine analogs)
IT Potential barrier
(rotational, of thyroxine and triiodothyronine analogs)
IT 1678-72-4 37642-60-7 52050-08-5
RL: PRP (Properties)
(conformation of, mol. orbital energy calcn. in, thyroid hormone activity in relation to)
IT 51-48-9, properties 6893-02-3
RL: PRP (Properties)
(conformation of, mol. orbital energy calcns. in, biol. activity in relation to)
IT 56-41-7, properties 60-18-4, properties
RL: PRP (Properties)
(mol. orbital energies of)
IT 101-84-8 108-95-2, properties 123-31-9, properties 833-98-7 22040-02-4 28419-69-4 51930-03-1 51930-04-2
RL: PRP (Properties)
(rotational energy of)

=> d l45 5 all
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:y

AN 81:99798 CA
TI Hormonally active halogen free analogs of thyroxine
AU Jorgensen, E. C.; Frieden, E.; Block, P., Jr.
CS Sch. Pharm., Univ. California, San Francisco, CA, USA
SO Proceedings of the Western Pharmacology Society (1974), 17, 271-5
CODEN: PWPSA8; ISSN: 0083-8969
DT Journal
LA English
CC 2-3 (Hormone Pharmacology)
AB Synthesis of thyroid hormone analogs which contained no halogens showed that neither the halogen atoms nor the ether oxygen were essential features for appreciable thyroid hormone activity. Nonpolar groups of limited size and shape, as substituents adjacent to the connecting bridge (3 and 5 positions), provide the steric constraint which defines this semirigid structure. Specific polar groups, an anionic sidechain (1-position) and phenolic hydroxyl group (4'-position, are required at opposite ends of the central core. Activity of this basal structure is enhanced by a lipophiilic substituent adjacent to the phenolic group, and positioned distally in space to the nonphenolic ring. Since methylated analogs of thyroxine and triiodothyronine were active in the rat the concept of at least 2 active thyroid hormones was supported. The essential structure consisted of a central lipophilic core of 2 mutually perpendicular aromatic rings, insulated from each other and positioned at an angle of about 120.deg. by an appropriate bridging atom (O, C, or S).
ST thyroid hormone analog structure activity
IT Thyroid hormones
RL: BIOL (Biological study)
(analogs, biol. activity of, structure in relation to)
IT Molecular structure-biological activity relationship
(of thyroid hormone analogs)
IT 2378-96-3 26384-44-1 30804-65-0 35897-89-3 37642-60-7 38896-90-1 52050-08-5
RL: BIOL (Biological study)
(as thyroid hormone analog)
IT 51-48-9, biological studies
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(biol. activity of)

AN 81:131122 CA
TI Thyroxine analogs. 22. Thyromimetic activity of halogen-free derivatives of 3,5-dimethyl-L-thyronine
AU Jorgensen, Eugene C.; Murray, Wallace J.; Block, Paul, Jr.
CS Sch. Pharm., Univ. California, San Francisco, CA, USA
SO Journal of Medicinal Chemistry (1974), 17(4), 434-9
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
CC 2-3 (Hormone Pharmacology)
Section cross-reference(s): 34
AB Of a series of 4 title compds. prepd. and tested in the rat antigoiter assay, 3,5-dimethyl-3'-isopropyl-L-thyronine (I) [26384-44-1] had 18% of the activity of L-thyroxine [51-48-9]. I was prepared from N-acetyl-3,5-diiodo-4-(4-methoxy-3-isopropylphenoxy)-L-phenylalanine Et ester [23241-32-9] by cyanation, hydrogenation, and HI cleavage of the methyl ether group. Activity in relation to replacement of halogen atoms on the thyronine nucleus by alkyl groups, and replacement of the central ether linkage by a methylene bridge is discussed. NMR and mass spectral data showed that compds. previously reported as as 3,5,3',5'-tetramethyl-DL-thyronine [26384-21-4] and 3,5-dimethyl-3'-isopropyl-DL-thyronine [26384-20-3] were isomers of those structures.
ST thyroxine alkyl analog goiter inhibitor; thyroid hormone alkyl thyronine
IT Thyroid hormones
RL: BIOL (Biological study)
(halogen-free dimethylthyronine derivs.)
IT Molecular structure-biological activity relationship
(thyromimetic, of dimethylthyronine derivs.)
IT 26384-21-4
RL: BIOL (Biological study)
(as structure for 3,5,3',5'-tetramethyl-DL-thyronine, NMR and mass spectrum in relation to)
IT 26384-20-3
RL: BIOL (Biological study)
(as structure for 3,5-dimethyl-3'-isopropyl-DL-thyronine, NMR and mass spectrum in relation to)
IT 23241-32-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyanation of)
IT 35897-90-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(iodination of)
IT 10024-90-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidn. and hydrolysis of)
IT 26384-44-1P 26384-50-9P 52050-08-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and thyromimetic activity of)
IT 14786-82-4P 29358-99-4P 52498-34-7P 52498-35-8P 52498-36-9P
52498-37-0P 52498-38-1P 52498-39-2P 52498-40-5P 52777-31-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 35897-89-3 37642-60-7
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(thyromimetic activity of)
IT 51-48-9, biological studies
RL: BIOL (Biological study)
(thyromimetic activity of halogen-free dimethylthyronine derivs. in relation to)

AN 81:146096 CA
TI Thyromimetic activity of methylthyronines in the bullfrog tadpole
AU Frieden, Earl; Yoshizato, Katsutoshi
CS Dep. Chem., Florida State Univ. , Tallahassee, FL, USA
SO Endocrinology (1974), 95(1), 188-94
CODEN: ENDOAO; ISSN: 0013-7227
DT Journal
LA English
CC 2-4 (Hormone Pharmacology)
Section cross-reference(s): 12
AB On injection into bullfrog tadpole, 3'-isopropyl-3,5-dimethylthyronine (I) [26384-44-1] had 20-25% of the activity of L-thyroxine [51-48-9] when compared for effects on urea excretion and percent tail decrease. 3,5,3'-Trimethylthyronine [52050-08-5] and 3,5,3',5'-tetramethylthyronine [35897-89-3] showed .sim.15% of the activity of thyroxine. 3,5-Diiodo-4-(3',5'-diiodo-4'-hydroxybenzyl)-DL-phenyl acetic acid [38960-79-1] and 3,5-diiodo-4-(3'-iodo-4'-hydroxybenzyl)-DL-phenylalanine [37642-60-7] were equal to or slightly more active than the corresponding oxyether compd. The chem. structure required for a thyromimetic response consists of a central lipophilic core, sterically constrained by bulky 3,5,3'-substituents with 2 specific anionic groups, located at the distal ends of the mol. Apparently, neither the halogens nor the ether oxygen are essential features for significant thyroid hormone activity.
ST methylthyronine thyroid hormone tadpole
IT Thyroid hormones
RL: BIOL (Biological study)
(methylthyronine as)
IT Molecular structure-biological activity relationship
(thyromimetic, of methylthyronines)
IT L-Tyrosine, O-(4-hydroxy-3,5-diiodophenyl)-3,5-diiodo-, analogs
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(thyromimetic activity of)
IT 534-51-0 6893-02-3 26384-44-1 35897-89-3 35897-90-6 37642-60-7 38960-79-1 52050-08-5
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(thyromimetic activity of)

AN 84:69625 CA

TI Binding of selected iodothyronine analogs to receptor sites of isolated rat hepatic nuclei. High correlation between structural requirements for nuclear binding and biological activity

AU Koerner, Diona; Schwartz, Harold L.; Surks, Martin I.; Oppenheimer, Jack H.; Jorgensen, Eugene C.

CS Dep. Med., Montefiore Hosp. Med. Cent., Bronx, NY, USA

SO Journal of Biological Chemistry (1975), 250(16), 6417-23
CODEN: JBCHA3; ISSN: 0021-9258

DT Journal

LA English

CC 2-1 (Hormone Pharmacology)

AB The limited capacity, high affinity binding of 35 iodothyronine analogues by rat liver nuclei was examd. in an in vitro system. The in vitro nuclear binding of all the analogues tested was highly correlated with their published thyromimetic potencies in the intact animals. Binding and biol. activity were greater for 3'-mono- than 3',5'-di-substituted iodothyronines. A 4'-hydroxyl group was essential, but the 3' substituent could be several halogen or nonhalogen groups for which the distal conformation was preferred. The ether linkage could be replaced equally well by a methylene or sulfur group. The presence of both 3 and 5 groups which were limited to halogens or small alkyl groups were necessary for the maintenance of significant activity. Halogen-free iodothyronines had very low, but significant activity both in vitro and in vivo. The data provide information on the structural requirements for thyroid hormone action and further support the physiol. relevance of the nuclear sites.

ST iodothyronine receptor liver nucleus; structure activity iodothyronine thyromimetic

IT Receptors
RL: BIOL (Biological study)
(for thyroid hormones, of liver nucleus)

IT Cell nucleus
(iodothyronine binding by, of liver)

IT Thyroid hormones
RL: BIOL (Biological study)
(receptor for, of liver nucleus)

IT Liver
(thyroid hormone receptor of nucleus of)

IT Molecular structure-biological activity relationship
(thyromimetic, of iodothyronine analogs)

IT 51-23-0 51-48-9, biological studies 70-40-6 857-98-7 1041-01-6
2378-96-3 3272-50-2 3272-52-4 3415-06-3 4080-15-3 4299-63-2
4299-64-3 4299-87-0 4564-77-6 5383-39-1 6893-02-3 10439-94-8
10466-20-3 13724-85-1 17944-26-2 25119-48-6 26384-44-1
28619-63-8 30804-62-7 30804-65-0 35897-89-3 37642-60-7
38896-90-1 39693-06-6 51725-31-6 52050-08-5 58297-21-5
58297-22-6 58297-23-7 58297-24-8
RL: BIOL (Biological study)
(thyromimetic activity of, liver nucleus binding in relation to)

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     FILE 'USPATFULL, CAPLUS' ENTERED AT 10:55:48 ON 17 DEC 2003
               ACTIVATE L09980406/L
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L1              STR
L2   (         11)SEA FILE=REGISTRY SSS FUL L1
L3   (         30)SEA FILE=CAPLUS ABB=ON  PLU=ON  L2
L4   (         14)SEA FILE=CAPLUS ABB=ON  PLU=ON  L2/USES OR L2/BIOL
L5   (          0)SEA FILE=CAPLUS ABB=ON  PLU=ON  L4 AND HAIR
L6   (          0)SEA FILE=CAPLUS ABB=ON  PLU=ON  L4 AND THYROIDR
L7   (         13)SEA FILE=CAPLUS ABB=ON  PLU=ON  L4 AND THYROID
L8   (          0)SEA FILE=CAPLUS ABB=ON  PLU=ON  L4 AND ALOPECIA
L9   (          0)SEA FILE=CAPLUS ABB=ON  PLU=ON  L4 AND BALD?
L10  (          3)SEA FILE=USPATFULL ABB=ON  PLU=ON  L2
L11  (          2)SEA FILE=CAPLUS ABB=ON  PLU=ON  40487-99-8/BIOL
L12  (          0)SEA FILE=TOXCENTER ABB=ON  PLU=ON  40487-99-8/BIOL
L13  (          2)SEA 40487-99-8/BIOL
L14  (          2)SEA FILE=CAPLUS ABB=ON  PLU=ON  40487-99-8
L15  (          0)SEA FILE=TOXCENTER ABB=ON  PLU=ON  40487-99-8
L16  (          2)SEA 40487-99-8
L17  (          1)SEA FILE=CAPLUS ABB=ON  PLU=ON  27486-96-0
L18  (          0)SEA FILE=TOXCENTER ABB=ON  PLU=ON  27486-96-0
L19  (          1)SEA 27486-96-0
L20  (         12)SEA FILE=CAPLUS ABB=ON  PLU=ON  52050-08-5 OR 40487-99-8 OR L17
L21  (          1)SEA FILE=TOXCENTER ABB=ON  PLU=ON  52050-08-5 OR 40487-99-8 OR
L22  (         13)SEA 52050-08-5 OR 40487-99-8 OR L19
L23  (         10)SEA FILE=CAPLUS ABB=ON  PLU=ON  CARDIAC SPARING
L24  (          8)SEA FILE=USPATFULL ABB=ON  PLU=ON  CARDIAC SPARING
L25  (         18)SEA CARDIAC SPARING
L26  (         19)SEA FILE=CAPLUS ABB=ON  PLU=ON  CARDIAC (5A) SPARING
L27  (         35)SEA FILE=USPATFULL ABB=ON  PLU=ON  CARDIAC (5A) SPARING
L28  (         54)SEA CARDIAC (5A) SPARING
L29  (          4)SEA FILE=CAPLUS ABB=ON  PLU=ON  THYROID AND L26
L30  (          5)SEA FILE=USPATFULL ABB=ON  PLU=ON  THYROID AND L27
L31  (          9)SEA THYROID AND L28
L32  (          0)SEA FILE=CAPLUS ABB=ON  PLU=ON  L20 AND L26
L33  (          0)SEA FILE=USPATFULL ABB=ON  PLU=ON  L22 AND L27
L34  (          0)SEA L22 AND L28
L35  (          0)SEA FILE=CAPLUS ABB=ON  PLU=ON  L20 AND (CARDIAC)
L36  (          0)SEA FILE=USPATFULL ABB=ON  PLU=ON  L22 AND (CARDIAC)
L37  (          0)SEA L22 AND (CARDIAC)
L38  (          1)SEA FILE=CAPLUS ABB=ON  PLU=ON  L20 AND (HEART OR PRESSURE)
L39  (          0)SEA FILE=USPATFULL ABB=ON  PLU=ON  L22 AND (HEART OR PRESSURE)
L40  (          1)SEA L22 AND (HEART OR PRESSURE)
L41  (          1)SEA FILE=CAPLUS ABB=ON  PLU=ON  L20 AND (HEART OR PRESSURE)
L42  (          0)SEA FILE=TOXCENTER ABB=ON  PLU=ON  L21 AND (HEART OR PRESSURE)
L43  (          1)SEA L40
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     FILE 'REGISTRY, USPATFULL, CAPLUS' ENTERED AT 10:56:17 ON 17 DEC 2003
L44             1 FILE REGISTRY
L45            11 FILE REGISTRY

     FILE 'CAPLUS, USPATFULL, TOXCENTER' ENTERED AT 11:02:03 ON 17 DEC 2003
L46            30 FILE CAPLUS
L47             3 FILE USPATFULL
L48             5 FILE TOXCENTER
     TOTAL FOR ALL FILES
L49            38 S L45
L50             2 FILE CAPLUS
L51             0 FILE USPATFULL
L52             0 FILE TOXCENTER
     TOTAL FOR ALL FILES
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L53           2 S TRIMETHYLTHYRONINE
L54           4 FILE CAPLUS
L55           0 FILE USPATFULL
L56           1 FILE TOXCENTER
     TOTAL FOR ALL FILES
L57           5 S TRIMETHYL(3A)THYRONINE
L58       18002 FILE CAPLUS
L59        3924 FILE USPATFULL
L60        3208 FILE TOXCENTER
     TOTAL FOR ALL FILES
L61       25134 S (L-TYROSINE) OR (L(1W) TYROSINE)
L62          47 FILE CAPLUS
L63          33 FILE USPATFULL
L64           6 FILE TOXCENTER
     TOTAL FOR ALL FILES
L65          86 S L61 (5A) (DIMETHYL)
L66         100 FILE CAPLUS
L67         104 FILE USPATFULL
L68           9 FILE TOXCENTER
     TOTAL FOR ALL FILES
L69         213 S L61 (5A) (DIMETHYL?)
L70           5 FILE CAPLUS
L71           8 FILE USPATFULL
L72           1 FILE TOXCENTER
     TOTAL FOR ALL FILES
L73          14 S L69 (5A) (HYDROXY?)
L74       19717 FILE CAPLUS
L75        2175 FILE USPATFULL
L76        8512 FILE TOXCENTER
     TOTAL FOR ALL FILES
L77       30404 S 52050-08-5/RN OR ?THYRONINE? OR 52050-08-5
L78          61 FILE CAPLUS
L79         495 FILE USPATFULL
L80          38 FILE TOXCENTER
     TOTAL FOR ALL FILES
L81         594 S L77 AND (HAIR? OR ALOPECIA OR BALD?)

     FILE 'REGISTRY' ENTERED AT 11:09:46 ON 17 DEC 2003
L82           1 S THYRONINE/CN

     FILE 'CAPLUS, USPATFULL, TOXCENTER' ENTERED AT 11:10:13 ON 17 DEC 2003
L83           8 FILE CAPLUS
L84         436 FILE USPATFULL
L85           3 FILE TOXCENTER
     TOTAL FOR ALL FILES
L86         447 S L81 AND (METHYL?)
L87           9 FILE CAPLUS
L88         428 FILE USPATFULL
L89           5 FILE TOXCENTER
     TOTAL FOR ALL FILES
L90         442 S L81 AND (?METHYL)
L91          10 FILE CAPLUS
L92         445 FILE USPATFULL
L93           7 FILE TOXCENTER
     TOTAL FOR ALL FILES
L94         462 S L86 OR L90

     FILE 'REGISTRY' ENTERED AT 11:17:55 ON 17 DEC 2003
L95           1 S 6893-02-3/RN
                SET NOTICE 1 DISPLAY
                SET NOTICE LOGIN DISPLAY

     FILE 'CAPLUS, USPATFULL, TOXCENTER' ENTERED AT 11:19:00 ON 17 DEC 2003
L96       31768 FILE CAPLUS
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L97       58023 FILE USPATFULL
L98       11948 FILE TOXCENTER
     TOTAL FOR ALL FILES
L99      101739 S TRIIODOTHYRONINE OR (L-T3) OR (L(1W) T3) OR T3 OR (TRIIODO (5
L100    2550638 FILE CAPLUS
L101     873754 FILE USPATFULL
L102     497113 FILE TOXCENTER
     TOTAL FOR ALL FILES
L103    3921505 S SUBSTITUT? OR ALKYLAT? OR METHYL?
L104       1344 FILE CAPLUS
L105       1011 FILE USPATFULL
L106        437 FILE TOXCENTER
     TOTAL FOR ALL FILES
L107       2792 S L99 (2S) (L103 OR (FREE (3A) IODINE))
L108       1156 FILE CAPLUS
L109       1010 FILE USPATFULL
L110        348 FILE TOXCENTER
     TOTAL FOR ALL FILES
L111       2514 S L99 (1S) (L103 OR (FREE (3A) IODINE))
L112         14 FILE CAPLUS
L113          2 FILE USPATFULL
L114          9 FILE TOXCENTER
     TOTAL FOR ALL FILES
L115         25 S L99 (1S) ((FREE (3A) IODINE))

     FILE 'REGISTRY' ENTERED AT 11:28:03 ON 17 DEC 2003

     FILE 'CAPLUS, USPATFULL, TOXCENTER' ENTERED AT 11:28:06 ON 17 DEC 2003

     FILE 'REGISTRY' ENTERED AT 11:28:19 ON 17 DEC 2003

     FILE 'CAPLUS, USPATFULL, TOXCENTER' ENTERED AT 11:28:20 ON 17 DEC 2003

     FILE 'REGISTRY' ENTERED AT 11:28:26 ON 17 DEC 2003

     FILE 'CAPLUS, USPATFULL, TOXCENTER' ENTERED AT 11:28:28 ON 17 DEC 2003

     FILE 'REGISTRY' ENTERED AT 11:28:33 ON 17 DEC 2003

     FILE 'CAPLUS, USPATFULL, TOXCENTER' ENTERED AT 11:28:35 ON 17 DEC 2003

     FILE 'REGISTRY' ENTERED AT 11:28:41 ON 17 DEC 2003

     FILE 'CAPLUS, USPATFULL, TOXCENTER' ENTERED AT 11:28:42 ON 17 DEC 2003
L116          2 FILE CAPLUS
L117          1 FILE USPATFULL
L118          0 FILE TOXCENTER
     TOTAL FOR ALL FILES
L119          3 S L99 (1S) ((FREE (3A) HALOGEN?))
L120          2 FILE CAPLUS
L121          1 FILE USPATFULL
L122          0 FILE TOXCENTER
     TOTAL FOR ALL FILES
L123          3 S L119 NOT L115

     FILE 'USPATFULL, CAPLUS' ENTERED AT 11:40:44 ON 17 DEC 2003
L124        343 FILE USPATFULL
L125      17177 FILE CAPLUS
     TOTAL FOR ALL FILES
L126      17520 S 6893-02-3/RN OR 6893-02-3
L127      58067 FILE USPATFULL
L128      32491 FILE CAPLUS
     TOTAL FOR ALL FILES
L129      90558 S L99 OR L126
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L130          3 FILE USPATFULL
L131         99 FILE CAPLUS
     TOTAL FOR ALL FILES
L132        102 S L129 (2S) (FREE (5A) (HALOGEN OR IODO?))
L133          2 FILE USPATFULL
L134         99 FILE CAPLUS
     TOTAL FOR ALL FILES
L135        101 S L132 NOT 119
L136          2 FILE USPATFULL
L137         98 FILE CAPLUS
     TOTAL FOR ALL FILES
L138        100 S L135 NOT L115
                SAVE ALL L09980406/L
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L149 ANSWER 8 OF 11 MEDLINE on STN
AN 60055782 MEDLINE
DN 60055782
TI Effects of **methyl** group **substitution** for iodine on metabolic activity of thyroxine, **triiodothyronine** and tetraiodothyropropionic acid.
AU PITTMAN C S; SHIDA H; BARKER S B
SO Endocrinology, (1961 Feb) 68 248-52.
DT Journal
LA English
FS OLDMEDLINE
EM 196112
ED Entered STN: 19990716
Last Updated on STN: 19990716
ST basal metabolism - pharmacology; thyroxin - related compounds; tissue metabolism - pharmacology; triiodothyronine - related compounds
RN 51-48-9 (THYROXIN); 6893-02-3 (TRIIODOTHYRONINE)

L149 ANSWER 2 OF 11 EMBASE COPYRIGHT 2003 ELSEVIER INC. ALL RIGHTS RESERVED.
on STN DUPLICATE 2
AN 95198257 EMBASE
DN 1995198257
TI Synthesis and structure-activity relationships of oxamic acid and acetic acid derivatives related to L-thyronine.
AU Yokoyama N.; Walker G.N.; Main A.J.; Stanton J.L.; Morrissey M.M.; Boehm C.; Engle A.; Neubert A.D.; Wasvary J.M.; Stephan Z.F.; Steele R.E.
CS Research Department, Ciba Pharmaceuticals, 556 Morris Avenue,Summit, NJ 07901, United States
SO Journal of Medicinal Chemistry, (1995) 38/4 (695-707).
ISSN: 0022-2623 CODEN: JMCMAR
CY United States
DT Journal; Article
FS 030 Pharmacology
037 Drug Literature Index
LA English
SL English
AB Aryloxamic acids 7 and 23, (arylamino)acetic acids 29, arylpropionic acids 33, arylthioacetic acids 37, and (aryloxy)acetic acid 41 related to L-**triiodothyronine** (**L-T3**) were prepared and tested in vitro for binding to the rat liver nuclear **L-T3** receptor and the rat membrane **L-T3** receptor. The structure-activity relationships for these compounds are described, with 7f, 23a, 29c, 33a, 37b, and 41 showing excellent potency (IC50's of 0.19, 0.16, 1.1, 0.11, 3.5, and 0.10 nM, respectively) to the nuclear receptor and significantly lower binding affinity to the membrane receptor (IC50's > 5 .mu.M). Some of these compounds, especially in the oxamic acid series 7 and 23, showed an unprecedented potency for **methyl-substituted** derivatives such as 7f and 23a. Compounds 7f and 23a showed good lipid lowering effects in rats with ED50's of 20 and 5 .mu.g/kg po, respectively, and a lack of cardiac side effects in rats at doses as high as 10 and 25 mg/kg po, respectively.
CT Medical Descriptors:
animal cell
animal model
animal tissue
article
binding affinity
cardiotoxicity
controlled study
dose response
drug potency
drug synthesis
lipid blood level
male
nonhuman
oral drug administration
rat
structure activity relation
Drug Descriptors:
*liothyronine receptor
cell nucleus receptor
membrane receptor
*3,5 dibromo 3' (2,3 dihydro 3 oxo 6 pyridazinylmethyl)thyronine: PD, pharmacology
*3,5 dibromo 3' (2,3 dihydro 3 oxo 6 pyridazinylmethyl)thyronine: AN, drug analysis
*3,5 dibromo 3' (2,3 dihydro 3 oxo 6 pyridazinylmethyl)thyronine: CM, drug comparison
*3,5 dibromo 3' (2,3 dihydro 3 oxo 6 pyridazinylmethyl)thyronine: DV, drug development
*hypocholesterolemic agent: PD, pharmacology

*hypocholesterolemic agent: DV, drug development
*hypocholesterolemic agent: CM, drug comparison
*hypocholesterolemic agent: AN, drug analysis
*liothyronine: PD, pharmacology
[[4 [3 (4 fluoro alpha hydroxybenzyl) 4 hydroxyphenoxy] 3,5 dimethylphenyl]amino]oxoacetic acid ethyl ester: CM, drug comparison
[[4 [3 (4 fluoro alpha hydroxybenzyl) 4 hydroxyphenoxy] 3,5 dimethylphenyl]amino]oxoacetic acid ethyl ester: AN, drug analysis
[[4 [3 (4 fluoro alpha hydroxybenzyl) 4 hydroxyphenoxy] 3,5 dimethylphenyl]amino]oxoacetic acid ethyl ester: PD, pharmacology
[[4 [3 (4 fluoro alpha hydroxybenzyl) 4 hydroxyphenoxy] 3,5 dimethylphenyl]amino]oxoacetic acid ethyl ester: DV, drug development
cholesterol: EC, endogenous compound
n [3,5 dimethyl 4 (4 hydroxy 3 isopropylphenoxy)phenyl]oxamic acid: AN, drug analysis
n [3,5 dimethyl 4 (4 hydroxy 3 isopropylphenoxy)phenyl]oxamic acid: CM, drug comparison
n [3,5 dimethyl 4 (4 hydroxy 3 isopropylphenoxy)phenyl]oxamic acid: DV, drug development
n [3,5 dimethyl 4 (4 hydroxy 3 isopropylphenoxy)phenyl]oxamic acid: PD, pharmacology
unclassified drug

RN (3,5 dibromo 3' (2,3 dihydro 3 oxo 6 pyridazinylmethyl)thyronine) 105211-23-2; (liothyronine) 6138-47-2, 6893-02-3; (cholesterol) 57-88-5

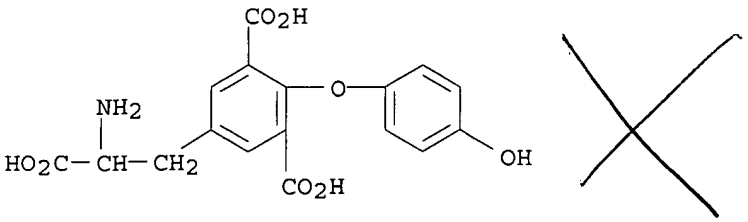
CN (1) L 94901

CO (1) Smith kline and french

L123 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN

AB The mol. conformation of the **halogen-free** thyroid hormone analog, N-acetyl-4'-methoxy-3,5,3'-trimethyl-L-thyronine Et ester, was detd. by x-ray diffraction techniques. The obsd. mol. conformation was similar to that found for the natural hormone 3,5,3'-**triiodo -L-thyronine** (**T3**). In this structure, the 3'-Me group is distal, the overall conformation is cisoid, and the di-Ph ether conformation is twist-skewed. These structural similarities with **T3** showed that the conformational features required by the active hormone can still be maintained with Me substitution. The observation that the **halogen-free** analogs have relatively high activity but extremely low protein binding affinity implies that the role of I in hormone transport and biol. activity can be differentiated. These data suggest that the I atoms enhance hormone-protein binding by virtue of their electronic, as well as steric, properties.

ACCESSION NUMBER: 1980:193090 CAPLUS
DOCUMENT NUMBER: 92:193090
TITLE: Role of iodine in thyroid hormones: molecular conformation of a halogen-free hormone analog
AUTHOR(S): Cody, Vivian
CORPORATE SOURCE: Med. Found. Buffalo, Inc., Buffalo, NY, 14203, USA
SOURCE: Journal of Medicinal Chemistry (1980), 23(5), 584-7
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English

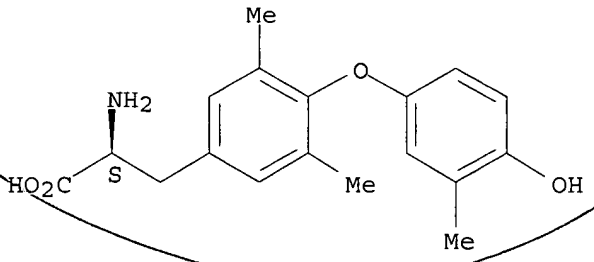


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L45 ANSWER 4 OF 11 REGISTRY COPYRIGHT 2003 ACS on STN
RN 52050-08-5 REGISTRY
CN L-Tyrosine, O-(4-hydroxy-3-methylphenyl)-3,5-dimethyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 3,5,3'-Trimethyl-L-thyronine
CN 3,5,3'-Trimethylthyronine
CN L-3,5,3'-Trimethylthyronine
FS STEREOSEARCH
MF C18 H21 N O4
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)

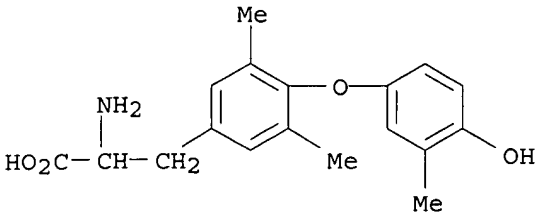
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)
9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L45 ANSWER 5 OF 11 REGISTRY COPYRIGHT 2003 ACS on STN
RN 40487-99-8 REGISTRY
CN Tyrosine, O-(4-hydroxy-3-methylphenyl)-3,5-dimethyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 3,5,3'-Trimethylthyronine
FS 3D CONCORD
DR 62960-43-4
MF C18 H21 N O4
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

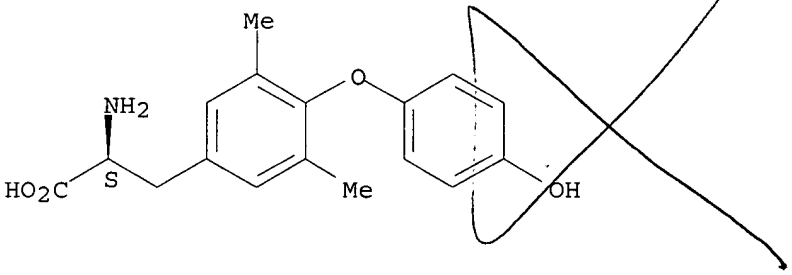


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L45 ANSWER 6 OF 11 REGISTRY COPYRIGHT 2003 ACS on STN
RN 35897-90-6 REGISTRY
CN L-Tyrosine, O-(4-hydroxyphenyl)-3,5-dimethyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Alanine, 3-[4-(p-hydroxyphenoxy)-3,5-xylyl]- (7CI)
OTHER NAMES:
CN 3,5-Dimethyl-L-thyronine
CN L-3,5-Dimethylthyronine
FS STEREOSEARCH
MF C17 H19 N O4
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.

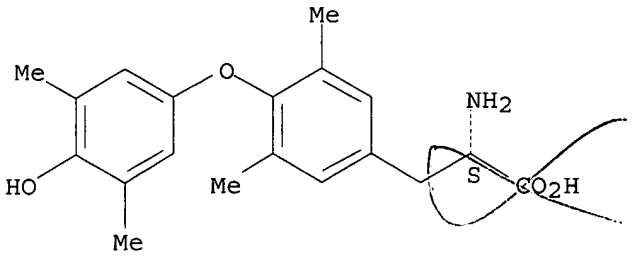


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L45 ANSWER 7 OF 11 REGISTRY COPYRIGHT 2003 ACS on STN
RN 35897-89-3 REGISTRY
CN L-Tyrosine, O-(4-hydroxy-3,5-dimethylphenyl)-3,5-dimethyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 3,5,3',5'-Tetramethyl-L-thyronine
CN 3,5,3',5'-Tetramethylthyronine
FS STEREOSEARCH
MF C19 H23 N O4
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

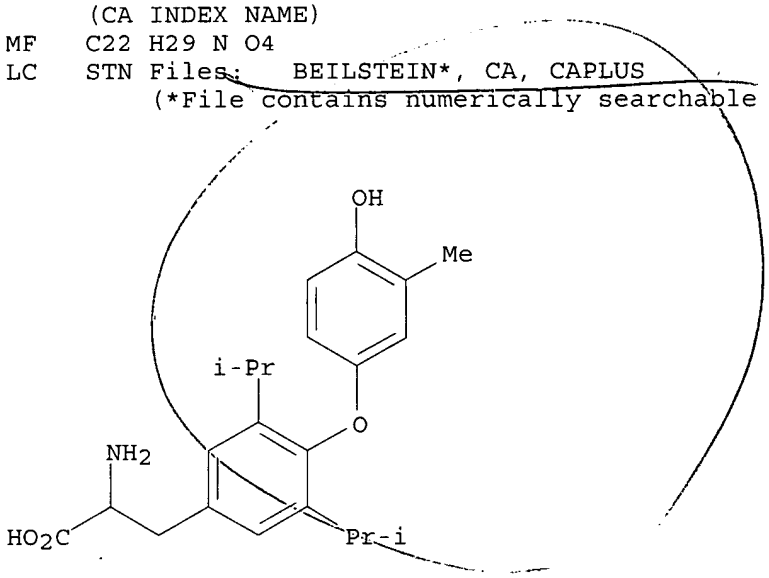
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

14 REFERENCES IN FILE CA (1907 TO DATE)
14 REFERENCES IN FILE CAPLUS (1907 TO DATE)

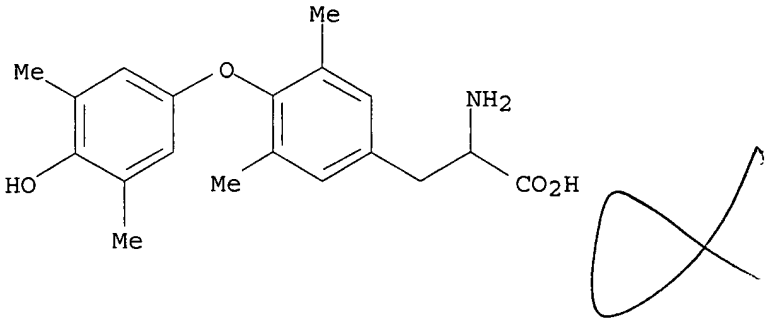
L45 ANSWER 8 OF 11 REGISTRY COPYRIGHT 2003 ACS on STN
RN 27486-96-0 REGISTRY
CN Alanine, 3-[4-[(4-hydroxy-m-tolyl)oxy]-3,5-diisopropylphenyl]-, DL- (8CI) (CA INDEX NAME)
MF C22 H29 N O4
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

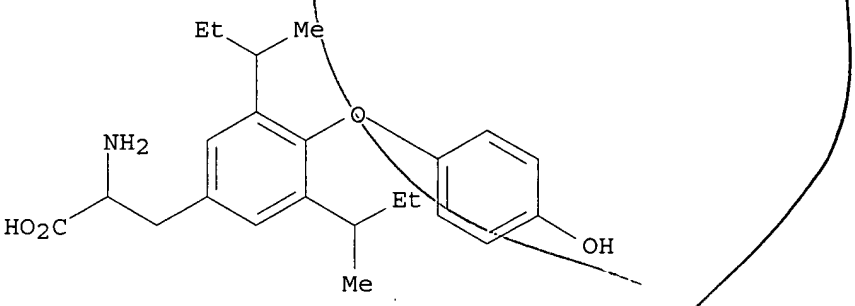
L45 ANSWER 9 OF 11 REGISTRY COPYRIGHT 2003 ACS on STN
RN 26384-21-4 REGISTRY
CN Tyrosine, O-(4-hydroxy-3,5-dimethylphenyl)-3,5-dimethyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Alanine, 3-[4-[(4-hydroxy-3,5-xylyl)oxy]-3,5-xylyl]- (6CI, 7CI)
CN Alanine, 3-[4-[(4-hydroxy-3,5-xylyl)oxy]-3,5-xylyl]-, DL- (8CI)
CN DL-Tyrosine, O-(4-hydroxy-3,5-dimethylphenyl)-3,5-dimethyl-
OTHER NAMES:
CN 3,5,3',5'-Tetramethyl-DL-thyronine
MF C19 H23 N O4
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE)
7 REFERENCES IN FILE CAPLUS (1907 TO DATE)
4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L45 ANSWER 10 OF 11 REGISTRY COPYRIGHT 2003 ACS on STN
RN 25849-86-9 REGISTRY
CN Tyrosine, O-(4-hydroxyphenyl)-3,5-bis(1-methylpropyl)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Alanine, 3-[3,5-di-sec-butyl-4-(p-hydroxyphenoxy)phenyl]-, DL- (8CI)
CN DL-Tyrosine, O-(4-hydroxyphenyl)-3,5-bis(1-methylpropyl)-
FS STEREOSEARCH
DR 25807-10-7
MF C23 H31 N O4
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

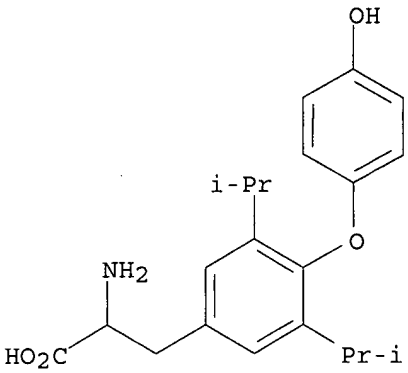


458. 10, 11

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L45 ANSWER 11 OF 11 REGISTRY COPYRIGHT 2003 ACS on STN
RN 19288-25-6 REGISTRY
CN Tyrosine, O-(4-hydroxyphenyl)-3,5-bis(1-methylethyl)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Alanine, 3-[4-(p-hydroxyphenoxy)-3,5-diisopropylphenyl]-, DL- (8CI)
CN DL-Tyrosine, O-(4-hydroxyphenyl)-3,5-bis(1-methylethyl)-
DR 25807-09-4
MF C21 H27 N O4
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)



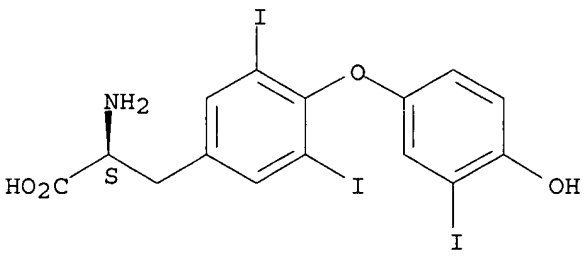
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=>

L95 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS on STN
RN **6893-02-3** REGISTRY
CN L-Tyrosine, O-(4-hydroxy-3-iodophenyl)-3,5-diiodo- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Alanine, 3-[4-(4-hydroxy-3-iodophenoxy)-3,5-diiodophenyl]-, L- (8CI)
CN Thyronine, 3,3',5-triiodo-, L- (6CI)
OTHER NAMES:
CN 3,3',5-Triiodo-L-thyronine
CN 3,3',5-Triiodothyronine
CN 3,5,3'-Triiodothyronine
CN 4-(4-Hydroxy-3-iodophenoxy)-3,5-diiodophenylalanine
CN L-3,3',5-Triiodothyronine
CN L-Liothyronine
CN L-T3
CN L-Triiodothyronine
CN Liothyronin
CN Liothyronine
CN NSC 80203
CN T3
CN T3 (amino acid)
CN T3 (Hormone)
CN Tresitope
CN Triiodo-L-thyronine
CN Triiodothyronine
FS STEREOSEARCH
DR 7013-53-8, 57164-27-9
MF C15 H12 I3 N O4
CI COM
LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMLIST, CIN, CSCHEM, CSNB, DDFU, DIOGENES, DRUGU, EMBASE, GMELIN*, HSDB*, IFICDB, IFIPAT, IFIUDB, IMSCOSEARCH, IPA, MEDLINE, MRCK*, NAPRALERT, NIOSHTIC, PROMT, RTECS*, SPECINFO, TOXCENTER, USAN, USPAT2, USPATFULL, VETU
(*File contains numerically searchable property data)
Other Sources: EINECS**, WHO
(**Enter CHEMLIST File for up-to-date regulatory information)

Absolute stereochemistry. Rotation (+).

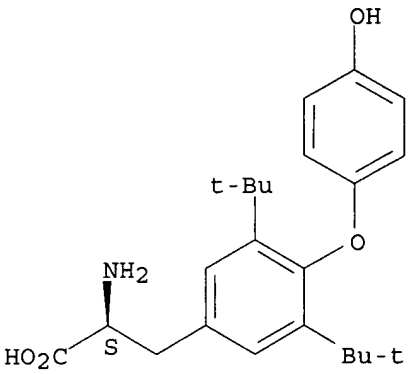


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

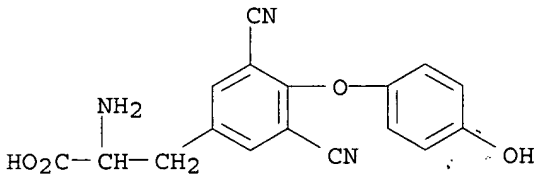
17162 REFERENCES IN FILE CA (1907 TO DATE)
143 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
17176 REFERENCES IN FILE CAPLUS (1907 TO DATE)
21 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L45 ANSWER 1 OF 11 REGISTRY COPYRIGHT 2003 ACS on STN
RN 439573-89-4 REGISTRY
CN L-Tyrosine, 3,5-bis(1,1-dimethylethyl)-O-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C23 H31 N O4
SR Reaction Database
LC STN Files: CASREACT

Absolute stereochemistry.



L45 ANSWER 2 OF 11 REGISTRY COPYRIGHT 2003 ACS on STN
RN 93326-20-6 REGISTRY
CN Alanine, 3-[3,5-dicyano-4-(p-hydroxyphenoxy)phenyl]- (7CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H13 N3 O4
LC STN Files: BEILSTEIN*, CAOLD
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L45 ANSWER 3 OF 11 REGISTRY COPYRIGHT 2003 ACS on STN
RN 93317-08-9 REGISTRY
CN Isophthalic acid, 5-(2-amino-2-carboxyethyl)-2-(p-hydroxyphenoxy)- (7CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H15 N O8
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS
(*File contains numerically searchable property data)